

Published Articles & Reports

[HYPERL INK "https: //doi.o rg/10.1 016/j.a tmosen v.2018. 05.053 "]	Foroutan, H., W. Tang, D. Heist, S. Perry, L. Brouwer, and E. Monbureau (2018) Numerical analysis of pollutant dispersion around elongated buildings: An embedded large eddy simulation approach. ATMOSPHERIC ENVIRONMENT. 187: 117-130; https://doi.org/10.1016/j.atmosenv.2018.05.053	CED	Peer Reviewed	ACE PEP- 1.8
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Impact / Purpose Statement

Published in the journal, Atmospheric Environment.

Product Description / Abstract

High fidelity, scale-resolving numerical simulations of flow and pollutant dispersion around several elongated isolated buildings are presented in this paper. The embedded large eddy simulation (ELES) is used to model flow and concentration fields for six test cases with various source-building geometries. Specifically, the influence of building aspect ratio, wind direction, and source location is examined with these cases. Results obtained from the present ELES model are evaluated using available wind tunnel measurements, including those of streamwise and spanwise velocities, turbulent kinetic energy, and streamwise, lateral, and spanwise pollutant concentrations. Comparisons indicate that the ELES provides realistic representations of the flow and concentration fields observed in wind tunnel experiments, and captures several complex phenomena including the lateral shift and enhanced descent of the plume for rotated/elongated buildings. Furthermore, the ELES provides a means to study the advective and turbulent concentration fluxes, plume shapes, and geometry of vortical structures that is used to examine turbulent transport of pollutants around buildings. We investigate the enhancement of vertical and lateral plume spread as the building aspect ratio is increased. In addition, through the study of advective and turbulent concentration fluxes, we shed light on the physics behind higher ground-level concentrations observed for rotated buildings.

Submitted

ORD-026535	Kostich, M., D. Bencic, A. Batt, M. See, R. Flick, D. Gordon, J. Lazorchak, and A. Biales. Multigene biomarkers of pyrethroid exposure: exploratory experiments. AQUATIC TOXICOLOGY.	EMMD	Peer Reviewed	SSWR 3.02C
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Impact / Purpose Statement

Submitted to the journal, Aquatic Toxicology.

Product Description / Abstract

We describe early development of transcript-profiling-based assays for detecting pyrethroid pesticides in water. We conducted 48-hour flow-through exposures of *Daphnia magna*, *Pimephales promelas* adults and *P. promelas* larvae to eight nominal concentrations of each of four pyrethroid insecticides (bifenthrin, cypermethrin, esfenvalerate, and permethrin). Concentration-response curves suggest steep dose responses, and LC50s below most published values. Expression microarray analysis of dissected brains from *P. promelas* adults and *P. promelas* whole larvae suggests transcript profiling of either biomaterial can be used to detect pyrethroids at concentrations well below *P. promelas* LC50s, and below LC50s of about 70% of aquatic species. Gene set analysis (GSA) highlighted several GO terms that can be rationalized based on known pyrethroid action, but implications of other implicated GO terms are unclear. However, GSA results were very sensitive to methodological variation. This work suggests that even without elucidating physiological networks, transcript profiling of *P. promelas* larvae can be used to detect pyrethroid pesticides with sufficient sensitivity to protect a broad range of aquatic species.

ORD-026708	Linkov, I., B. Trump, E. Anklam, D. Berube, P. Boisseau, C. Cummings, S. Ferson, M. Florin, B. Gldstein, D. Hristozov, K. Alstrup Jensen, G. Katalagarianakis, J. Kuzma, J. Lambert, T. Malloy, O. Malsch, A. Marcomini, M. Merad, J. Palma-Oliveira, E. Perkins, O. Renn, T. Seager, V. Stone, D. Vallero, and T. Vermeire. Science and Practice of Risk Policy and Governance for Emerging Technologies. Environment Systems & Decisions.	SED	Peer Reviewed	CSS 18.03.01
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Impact / Purpose Statement

Submitted to the journal, Environment Systems & Decisions.

Product Description / Abstract

This paper argues for a risk governance approach that integrates quantitative experimental information alongside qualitative expert insight to characterize and balance the risks, benefits, costs, and societal implications of emerging technologies.

ORD-026263	Zhen, H., D. Ekman, T. Collette, S. Glassmeyer, M. Mills, E. Furlong, D. Kolpin, and Q. Teng. Assessing the Impact of Wastewater Treatment Plant Effluent on Downstream Drinking Water-Source Quality Using a Zebrafish (Danio Rerio) Liver Cell-Based Metabolomics Approach. WATER RESEARCH.	EMMD	Peer Reviewed	SSWR 6.02B
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Impact / Purpose Statement

Submitted to the journal, Water Research.

Product Description / Abstract

Cell-based metabolomics was used in a proof-of-concept fashion to investigate the biological effects of contaminants as they traveled from a wastewater treatment plant (WWTP) discharge to a drinking water treatment plant (DWTP) intake in a surface water usage cycle. Zebrafish liver (ZFL) cells were exposed to water samples collected along a surface water flowpath, where a WWTP was located ~14.5 km upstream of a DWTP. The sampling sites included: 1) upstream of the WWTP, 2) the WWTP effluent discharging point, 3) a proximal location downstream of the WWTP outfall, 4) a distal location downstream of the WWTP outfall, 5) the drinking water intake, and 6) the treated drinking water collected prior to discharge to the distribution system. After a 48-hour laboratory exposure, the hydrophilic and lipophilic metabolites in ZFL cell extracts were analyzed by proton nuclear magnetic resonance (1H NMR) spectroscopy and gas chromatography-mass spectrometry (GC-MS), respectively. Multivariate statistical analysis revealed distinct changes in metabolite profiles in response to WWTP effluent exposure. These effects on the hydrophilic metabolome gradually diminished downstream of the WWTP, becoming non-significant at the drinking water intake (comparable to upstream of the WWTP). However, effects on the lipophilic metabolome increased significantly as the river flowed from the distal location downstream of the WWTP to the drinking water intake, suggesting a source of contamination in this watershed other than the WWTP. ZFL cells exposed to treated drinking water did not exhibit significant changes in either the hydrophilic or lipophilic metabolome (compared to the upstream site), suggesting that constituents in the WWTP effluent were efficiently removed by the drinking water treatment process. Impacts on ZFL cells from the WWTP effluent included disrupted energy metabolism, a global decrease in amino acids and altered lipid metabolism pathways. Overall, this study demonstrated the utility of cell-based metabolomics as an effective tool for assessing the biological effects of complex pollutant mixtures, particularly when used as a complement to conventional chemical monitoring.

Presentations

ORD-026746	Dugan, N., and B. Schaeffer. Overview of HABs Research Program - presentation, 5/29/18. To be presented at National Institute of Water Resource Directors, Research Triangle Park, North Carolina, USA, 05/29/2018 - 05/29/2018.	EMMD	Presentation	SSWR 4.01A
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Impact / Purpose Statement

Cleared by NRMRL

Presented at the National Institute of Water Resource Directors, Research Triangle Park, North Carolina, USA, 05/29/2018 - 05/29/2018.

Product Description / Abstract

This presentation is an overview of the cyanobacteria/harmful algal blooms research currently being performed within the Office of Research and Development's Safe and Sustainable Water Resources research program. The presentation highlights results in the following areas: lake monitoring for cyanobacteria toxins, remote sensing of cyanobacterial blooms, removal of toxins by activated carbon, health effects of microcystin congeners, validation studies of rapid PCR tests for toxin producing cyanobacteria, and analytical methods for toxin analysis in fish tissues.

ORD-024160	Linnenbrink, M., A. Guiseppi-Elie, P. Wong, and A. Ragin_Wilson. Characterizing Exposures to Tire Crumb Rubber Used on Synthetic Turf Playing Fields. To be presented at APHL, Pasadena, CA, USA, 06/02/2018 - 06/05/2018.	NERL IO	Presentation	N/A
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Impact / Purpose Statement

Cleared by OSP

Presented at the APHL, Pasadena, CA, USA, 06/02/2018 - 06/05/2018.

Product Description / Abstract

Tire crumb is a unique material requiring significant methods development for sampling the material and both chemical and biological analyses. The results of these studies are used to help inform exposure assessment for users of these fields.

ORD-026581	Price, P. Risk assessments for mixtures: technical methods commonly used in the United States. Presented at Advancing the Assessment of Chemical Mixtures and their Risks for Human Health and the Environment, Ispra, NA, ITALY, 05/29/2018 - 05/30/2018.	CED	Presentation	HHRA 3.232
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Impact / Purpose Statement

Presented at the Advancing the Assessment of Chemical Mixtures and their Risks for Human Health and the Environment, Ispra, NA, ITALY, 05/29/2018 - 05/30/2018.

Product Description / Abstract

A brief (20 minute) talk on the technical approaches used by EPA and other US agencies to assess risks posed by combined exposures to one or more chemicals. The talk systemically reviews the methodologies (whole-mixtures and component-based approaches) that are or have been used by EPA. Efforts are made to make the information understandable to the audience by using both U.S. figures and terminology and where appropriate to also use figures and terms in common use in the European Union.

ORD-025231	Singh, R., A. Chao, X. Xia, D. Shea, J. Sobus, and E. Ulrich. Improving High Throughput Exposomics through EPA's Non-Targeted Analysis Collaborative Trial (ENTACT). To be presented at American Society for Mass Spectrometry conference, San Diego, CA, USA, 06/03/2018 - 06/07/2018.	EMMD	Presentation	CSS 16.02.0 1
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Impact / Purpose Statement

Presented at the American Society for Mass Spectrometry conference, San Diego, CA, USA, 06/03/2018 - 06/07/2018.

Product Description / Abstract

Introduction

Humans are exposed to a myriad of chemicals on a daily basis. Fast, accurate and comprehensive analytical methods are needed to assess chemical exposures and protect human health. Recent applications of high resolution mass spectrometry (HRMS) and non-targeted analysis (NTA) have demonstrated the breadth of compounds that are present in the environment and living organisms. It has proven challenging, however, to confirm detected chemicals, and understand the chemical space limitations of the methods without extensive controlled experiments. To better assess NTA methods as tools for exposomics research, the US EPA's Non-Targeted Analysis Collaborative Trial (ENTACT) was initiated.

Methods

Ten different ENTACT mixtures were prepared using ~1200 chemicals from EPA's ToxCast program. ENTACT mixtures were analyzed using both positive and negative mode HRMS with atmospheric pressure chemical ionization (APCI) and electrospray ionization (ESI). Mixtures were further evaluated across two chromatographic methods: one using a C8 column with methanol as the organic modifier, and the other using a C18 column with acetonitrile.

Preliminary Data

ESI vs. APCI: The experiment comparing ionization sources showed that some compounds prefer a specific ionization source, with 193 correctly identified via APCI, 746 via ESI, and 104 via both methods. Given these findings, we conclude that complementary approaches, combining both APCI and ESI, should be routinely used for exposomics studies. These results are now being used to predict the ionization behavior of untested chemicals to improve the chances of applying successful methods. Models based on these data are further being used to select across tentatively identified candidate structures in various NTA applications. While it is easy to assume that formation of the $[M+H]^+$ is the predominant ionization mechanism, $[M]^+$ formation was observed to be significant in APCI data interpretation. The results of this research highlight the need to carefully interpret HRMS data.

C8/Methanol vs. C18/Acetonitrile: By changing the chemistry of the column packing material, increased interaction of the analytes with the column was observed, minimizing elution of analytes right after void volume. Furthermore, general improvement in ionization efficiency, peak shape, and analyte signal-to-

noise ratio was achieved by switching the organic modifier from methanol to acetonitrile. This in turn, enhanced the number of compounds that were identified with high confidence based on MS-only and MS/MS information and database matching. For one of the mixtures, the blinded true positive rate went from 13% to 42% by switching the analysis from the C8/Methanol to the C18/Acetonitrile method.

Novel Aspect

ENTACT uses ~1200 compounds with varying physico-chemical properties to allow comparison of ionization and separation modes for NTA methods.

ORD-025533	Theregowda, R., A. Gonzaacutetez-Mejiaacute;a , C. Ma, and J. Garland. Comparative Emergy Evaluation of Nutrient Recovery Technologies as an Alternative to Traditional Fertilizers and Nutrient Removal Technologies - abstract, 6/3/18. To be presented at New England Water Environment Association (NEWEA) 2018 Spring Meeting, New Port, Rhode Island, USA, 06/03/2018 - 06/06/2018.	SED	Presentation	SSWR 6.03A
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Impact / Purpose Statement

Cleared by NRMRL

Presented at the New England Water Environment Association (NEWEA) 2018 Spring Meeting, New Port, Rhode Island, USA, 06/03/2018 - 06/06/2018.

Product Description / Abstract

None

ORD-026827	Theregowda, R., A. Gonzalez-Mejia, J. Garland, and C. Ma. Nutrient recovery from municipal wastewater for sustainable food production systems: An alternative to traditional fertilizers - presentation, 6/3/18. To be presented at NEWEA Spring Meeting 2018, Newport, Rhode Island, USA, 06/03/2018 - 06/06/2018.	SED	Presentation	SSWR 6.03A
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Impact / Purpose Statement

Cleared by NRMRL

Presented at the New England Water Environment Association (NEWEA) 2018 Spring Meeting, New Port, Rhode Island, USA, 06/03/2018 - 06/06/2018.

Product Description / Abstract

None

ORD-024908	Willison, S., D. Stout, A. Mysz, J. Starr, D. Tabor, B. Wyrzykowska-Ceradini, E. Morris, J. Nardin, and E. Snyder. The Impacts of Wipe Sampling Variables on Method Performance for Hazardous Pesticide Environmental Samples [HS7.53.01-044]. To be presented at American Society of Mass Spectrometry, San Diego, CA, USA, 06/03/2018 - 06/08/2018.	EMMD	Poster	HS 7.53.01
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Impact / Purpose Statement

Presented at the American Society for Mass Spectrometry conference, San Diego, CA, USA, 06/03/2018 - 06/07/2018.

Product Description / Abstract

Poster -- Investigating the impacts of wipe sampling variables on pesticide surface recovery results and method performance

ORD-026643	Zartarian, V. Overview of EPA Office of Research and Development Lead (Pb) Science. To be presented at EPA Science Advisory Board Meeting, Washington, DC, USA, 06/01/2018 - 06/01/2018.	SED	Presentation	SHC 2.63.2
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Impact / Purpose Statement

High Profile

Presented at the Fire Continuum Conference, Missoula, MT, USA, 05/21/2018 - 05/24/2018.

Product Description / Abstract

Problem: Estimate children's blood lead levels (BLLs) for the U.S. residential population, given multimedia exposures from drinking water, soil, dust, air, and food

Stakeholders: EPA Office of Water and other Program Offices, public health community

Approach:

- Probabilistic analysis using coupled EPA's SHEDS Multimedia and IEUBK models
- Model evaluation using CDC NHANES BLLs data
- Determined relationship between daily average drinking water Pb concentrations & BLLs for specified scenarios
- Quantified relative exposure pathway contributions across population distributions
- Identified most important factors affecting BLLs